PROJECT **facts**

DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY

ADVANCED Resource

THE UNIVERSITY COAL RESEARCH PROGRAM

Sustaining a National program of university research in fundamental coal studies

The University Coal Research (UCR) Program began in 1979. Each year, following a nationwide competition, the U.S. Department of Energy's Office of Fossil Energy selects the 20 to 25 university-proposed projects out of more than 200 proposals that offer the best prospects for advancing coal science. Preference is given to projects that seek to improve the environmental compatibility of advanced coal concepts.

The grants range from $80,000 to $400,000 (DOE funding) for projects that generally take up to three years to complete. Often the Federal grants are supplemented by the fossil-energy industry. Research topics range from fundamental aspects of coal structure to carbon dioxide capture and disposal. Since the program's inception, 477 research projects have been supported, representing more than $81 million in Federal funding.

Fiscal Year 1996 will see 92 ongoing UCR projects funded for about $5 million. In 1995 private industry provided $1.34 million for the UCR Program.

Description of 1995 Winning Projects

- **University of Akron**, Akron, OH: a 36-month $199,965 grant for "In-Situ Infrared Study of Catalytic Decomposition of NO." Dr. S. Chuang will use an innovative infrared reactor system to study (1) the reactivity of adsorbates for direct NO decomposition using silanation to stabilize metal crystallites, support Cu-ZSM-5 catalyst, and promote Pt catalyst; and (2) improving catalyst activity and resistance to sintering, using oxygen spillover and desorption to enhance NO decomposition activity. The results will provide a basis for developing an effective catalyst for practical NO decomposition.

- **Auburn University**, Auburn, AL: a 36-month $197,237 grant for "Hindered Diffusion of Asphaltenes at Elevated Temperature and Pressure." Dr. J. Guin will investigate asphaltene diffusion in actual catalyst pores under elevated temperature and pressure conditions representative of catalytic upgrading. The results will provide a better understanding of the process for catalytically upgrading the first-stage heavy liquids necessary for obtaining clean transportation fuels from direct coal liquefaction processes.

- **Brigham Young University (BYU)**, Provo, UT: a 36-month $198,264 grant for "Determination of the Forms of Nitrogen Released in Coal Tar During Rapid Devolatilization." Dr. T. Fletcher will investigate the forms of nitrogen in coal, char, and tar that lead to nitrogen release during devolatilization, with analysis via nuclear magnetic resonance, x-ray photoelectron spectroscopy, and high-resolution nitrogen-specific chromatography. This research will provide (1) nitrogen release parameters during devolatilization for specific coals pertinent to the HIPPS and LEBS projects; (2) better fundamental understanding of the chemistry of nitrogen release; and (3) a nitrogen release submodel based on fundamental chemistry that may be more widely applicable than existing empirical relationships.

- **Brigham Young University (BYU)**, Provo, UT: a 36-month $199,926 grant for "Temperature, Velocity and Species Profile Measurements for Reburning & Advanced Reburning in a Pulverized, Entrained Flow, Coal Combustor." Dr. D. Tree will evaluate species, velocity, and temperature in a 0.5-Mw down-fired, pulverized-coal reactor.

WINNING PROJECTS ($ Total Cost)

University of Akron
Akron, OH
In-Situ Infrared Study of Catalytic Decomposition of NO
$266,620

Auburn University
Auburn, AL
Hindered Diffusion of Asphaltenes at Elevated Temperature and Pressure
$254,682

Brigham Young University
Provo, UT
Determination of the Forms of Nitrogen Released in Coal Tar During Rapid Devolatilization
$385,522

Brigham Young University
Provo, UT
Temperature, Velocity, and Species Profile Measurements for Reburning & Advanced Reburning in a Pulverized, Entrained Flow, Coal Combustor
$290,537

Brown University
Providence, RI
Char Crystalline Transformations During Coal Combustion and Their Implications for Carbon Burnout
$235,000

University of Cincinnati
Cincinnati, OH
Chemistry of Mercury Species and Their Control in Coal Combustion Environments
$246,280

WINNING PROJECTS (cont.) ($ Total Cost)

Clark Atlanta University
Atlanta, GA
Surface Modified Coals for Enhanced Catalyst Dispersion and Liquefaction
$200,000

Clark Atlanta University
Atlanta, GA
Low Temperature VOC Combustion over Manganese and Zinc $AlPO_4$ Molecular Sieves
$140,000

University of Hawaii at Manoa
Honolulu, HI
Laboratory Experiments to Simulate CO_2 Ocean Disposal
$318,195

Iowa State University
Arnes, IA
A Novel Approach to Catalytic Desulfurization of Coal
$200,000

University of Kentucky Research Foundation
Lexington, KY
A Silica/Fly Ash Based Technology for Controlling Pyrite Oxidation
$161,786

Lehigh University
Bethlehem, PA
Cermet Composite Thermal Spray Energy Coatings for Erosion and Corrosion Protection in Combustion Environments of Advanced Coal-Fired Boilers
$387,282

Lehigh University
Bethlehem, PA
Wet Solids Flow Enhancement
$222,193

Massachusetts Institute of Technology
Cambridge, MA
The Scale-up of Large Pressurized Fluidized Beds for Advanced Coal-Fired Power Processes
$562,000

University of Michigan
Ann Arbor, MI
Coal Conversion Wastewater Pretreatment by Catalytic Oxidation in Supercritical Water
$226,354

The research includes (1) modifying an existing pulverized-coal reactor for reburning and advanced reburning; (2) analyzing CO, CO_2, O_2, N_2, NOx, HCN, and NH_3, at several combustor positions; and (3) measuring intermediate species such as NH_3, NH, CH, and OH by planar laser-induced flourescence.

• **Brown University**, Providence, RI: a 36-month $200,000 grant for "Char Crystalline Transformations During Coal Combustion and Their Implications for Carbon Burnout." To optimize high carbon burnout in entrained-flow combustion systems, Dr. R. Hurt will use a new thermal-treatment apparatus, microthermography, and high-resolution-transmission electron microscopy fringe imaging, studying (1) the first kinetic thermal deactivation at peak particle temperatures equivalent in commercial pulverized coal-fired boilers; (2) the effect of the thermal treatment on carbon crystalline structure and its relationships with reactivity; and (3) the design and operation of pulverized coal-fired boilers for high carbon burnout.

• **University of Cincinnati**, Cincinnati, OH: a 36-month $196,046 grant for "Chemistry of Mercury Species and Their Control in Coal Combustion Environments." Dr. P. Biswas will investigate the chemistry of mercury and species formed during coal combustion. This project studies (1) the fate of mercury in high-temperature oxidizing environments with other species such as sulfur and chlorine; (2) in-situ laser-induced fluorescence and elastic light-scattering measurements during coal combustion, and (3) vapor-phase sorbent precursors for converting the mercury to the particulate phase. Results will provide cost-effective mercury-emission control.

• **Clark Atlanta University**, Atlanta, GA: a 36-month $200,000 grant for "Surface Modified Coals for Enhanced Catalyst Dispersion and Liquefaction" to investigate the dispersion of organic-soluble iron, molybdenum acetylacetonate, and carbonyls in coal prior to liquefaction. Dr. G. Abosti will use electrophoretic mobility technique, FT-IR, x-ray diffraction, demineralized, and surfactant-treated coals.

• **Clark Atlanta University**, Atlanta, GA: a 24-month $140,000 grant for "Low Temperature VOC Chemistry Combustion over Manganese and Zinc $AlPO_4$ Molecular Sieves". Dr. R. Szostak will examine manganese, cobalt, and zinc, containing aluminophosphates ($AlPO_4$) with large-pore (MeAPO-36 and -46) topologies, for the removal of low levels of VOCs from gas streams.

• **University of Hawaii at Manoa**, Honolulu, HI: a 36-month $299,971 grant for "Laboratory Experiments to Simulate CO_2 Ocean Disposal," assessing deep-ocean disposal of anthropogenic CO_2. Dr. S. Masutani will explore (1) hydrates and CO_2 dissolution into seawater at moderate (less than 1,000-m) depths and (2) any hazards to the marine environment by concentrated-point discharge of pure CO_2 effluent. The resulting predictive model is needed to assess CO_2 sequestration and environmental hazards and to ensure rapid dissolution.

• **Iowa State University**, Ames, IA: a 36-month $200,00 grant for "A Novel Approach to Catalytic Desulfurization of Coal." Dr. J. Verkade will investigate (1) a novel catalytic hydrodesulfurization process for removing organic and inorganic sulfur from coal; (2) the catalytic role of FE_{3+} for quantitative removal of sulfur from dibenzothiophene by PR_3; and (3) the removal of organic sulfur from petroleum feed-stocks by using water-soluble phosphines and solid-supported phosphines.

• **University of Kentucky Research Foundation**, Lexington, KY: a 24-month $139,782 grant for "A Silica/Fly-Ash-Based Technology for Controlling Pyrite Oxidation." Dr. Evangelou will evaluate how sodium metasilicate can produce a more effective silica coating than the coatings formed by flyash as the silica source.

• **Lehigh University**, Bethlehem, PA: a 36-month $199,993 grant for "Wet Solids Flow Enhancement." Dr. Caram will study the modification of coal surface properties to change the contact angle in the pendular bridges for inducing repulsive forces and water agglomeration. The study examines (1) the effect of changing the surface properties using silazanes and other chemicals and of particle-size distribution on the mechanical properties of coal; (2) the water distribution in the sample, with high-resolution-imaging NMR, and (3) the flow properties of wet coal, using a near-two-dimensional hopper with adjustable discharge orifice and wall angles.

• **Lehigh University**, Bethlehem, PA: a 36-month $188,497 grant for "Cermet Composite Thermal Spray Energy Coatings for Erosion and Corrosion Protection in Combustion Environments of Advanced Coal-Fired Boilers." Dr. A. Marder will investigate sprayed cermet coatings to determine the optimum ceramic/metal combination for erosion and corrosion resistance in advanced coal-fired boilers. The research includes (1) preparing model cermet and thermal spray coatings; (2) simulated erosion testing with boiler flyash as erodent; (3) corrosion testing by gaseous oxidation furnace studies and solid state diffusion couple sulfidation studies; and (4) characterizing the microstructure of all coatings by light optical microscopy, quantitative image analysis, scanning electron microscopy, electron probe microanalysis, and x-ray diffraction.

• **Massachusetts Institute of Technology**, Cambridge, MA: a 36-month $400,000 grant for "The Scale-up of Large Pressurized Fluidized Beds for Advanced Coal-Fired Power Processes." Dr. L. Glicksman will investigate the fluid dynamics, heat transfer, and solid capture of a large pressurized coal-fired unit, simulating a cold laboratory model of the flow in the "Four Rivers" Pressurized Circulating Fluidized Bed Combustor. Findings will be incorporated in the design of the Four Rivers power plant to be constructed under the aegis of the DOE's Clean Coal V, and will provide information for scaling up large pressurized fluidized beds in existing pilot plants.

• **University of Michigan**, Ann Arbor, MI: a 36-month, $200,000 grant for "Coal Conversion Wastewater Pretreatment by Catalytic Oxidation in Supercritical Water." Dr. P. Savage will investigate the catalytic mechanism and kinetics of organic pollutants responsible for oxidizing phenol and related compounds in supercritical waters.

• **University of New Mexico**, Albuquerque, NM: a 36-month $199,999 grant for "Slurry Phase Iron Catalysts for Indirect Coal Liquefaction," Dr. A. Datye will study the interaction between active iron phase catalysts and binder, using transmission electron microscopy and spectroscopy. The goal is to produce novel slurry phase iron catalysts that can meet DOE requirements for bubble column reactors.

• **North Carolina A&T State University**, Greensboro, NC: a 36-month $199,991 grant for "High Temperature High Pressure Thermodynamic Measurements for Coal Model Compounds." Dr. V. Kabadi will (1) quantitate four binary systems of coal model compounds using a high-temperature, high-pressure-flow vapor-liquid equilibrium (VLE) apparatus; and (2) determine enthalpies and heat capacities of coal model compounds, using a high-temperature calorimeter. The study will provide a better understanding of the thermodynamic models for coal-derived fluids for accurately predicting VLE and heat capacities of high boiling-coal liquid fractions.

• **Pennsylvania State University**, University Park, PA: a 24-month $140,000 grant for "Optimization of Char for NOx Reduction." Dr. J. Phillips will use microcalorimetry and steady-state isotopic transient kinetic analyses to study the oxidation/reduction mechanism of catalyzed carbon NOx reduction for optimizing catalysts. Results will clarify the reaction mechanism during NOx reduction and the role of reactive carbon site C_f reactive C(O) surface intermediates, and stable C-O surface complexes.

• **University of Rochester**, Rochester, NY: a 36-month $200,000 grant for "Removal of H_2S and SO_2 by a $CaCO_3$ Based Sorbents at High Pressure." Dr. S. Sotirchos will investigate SO_2 and H_2S removal by $CaCO_3$-based sorbent in pressurized fluidized-bed coal combustors and also high-pressure gasifier. The investigative techniques include thermogravimetic reactivity experiments, gas adsorption, mercury porosimetry, effective diffusivity measurements, and electron microscopy to analyze models for variable diffusivity shrinking core, diffusion, reaction, and structure evolution in porous solids. The results will help improve sorbent utilization in high-pressure units.

• **University of Utah**, Salt Lake City, UT: a 36-month $199,941 grant for "Comprehensive Investigation of the Liberation Characteristics of Pyrite and Other Mineral Matter." Dr. R. King will examine the particle size of pyrite and other mineral matter from coals, and developing simulation models for coal cleaning plants.

• **Virginia Polytechnic Institute and State University**, Blacksburg, VA: a 36-month $200,000 grant for "Novel Carbide and Nitride Catalysts for Upgrading Coal Liquids."

WINNING PROJECTS (cont.) ($ Total Cost)

University of New Mexico
Albuquerque, NM
Slurry Phase Iron Catalysts for Indirect Coal Liquefaction
$199,999

North Carolina A&T State University
Greensboro, NC
High Temperature High Pressure Thermodynamic Measurements for Coal Model Compounds
$199,991

Pennsylvania State University
University Park, PA
Optimization of Char for NOx Reduction
$140,000

University of Rochester
Rochester, NY
Removal of H_2S and SO_2 by $CaCO_3$ Based Sorbents at High Pressure
$215,000

University of Utah
Salt Lake City, UT
Comprehensive Investigation of the Liberation Characteristics of Pyrite and Other Mineral Matter from Coal
$199,941

Virginia Polytechnic Institute and State University
Blacksburg, VA
Novel Carbide and Nitride Catalysts for Upgrading Coal Liquids
$291,814

University of Washington
Seattle, WA
Electrokinetic Densification of Coal Fines in Waste Ponds
$215,240

University of Washington
Seattle, WA
Reduction of Inherent Mercury Emissions in PC Combustion
$197,089

Washington University
St. Louis, MO
Novel Techniques for Slurry Bubble Column Hydrodynamics
$653,980

Yale University
New Haven, CT
Advanced Solids NMR Studies of Coal Structure and Chemistry
$225,000

Dr. S. T. Oyama will study a novel catalyst: supported transition metal carbides and nitrides for processing coal-derived liquids. This project examines (1) the new catalysts; (2) carbides and nitrides of Ti, V, Nb, No, W, and Fe support on Al_2O_3 and on activated carbon; (3) MO_2C single crystals, to clarify the reactivity of the catalyst in a trickle-bed reactor; (4) the catalyst with Auger electron spectroscopy, for near-surface composition; and (5) absorbed intermediates on the catalyst by diffuse-reflectance infrared spectroscopy. Results will show the degree of sulfidation of the surface, the propensity to deposit coke, and the binding energy of intermediates to the catalyst.

• **University of Washington**, Seattle, WA: a 36-month $199,840 grant for "Electrokinetic Densification of Coal Fines in Waste Ponds." Dr. E. Davis will design, scale up, and optimize an in-situ pollution-remediation process, with electrokinetic removal and densification of colloidal coal and minerals. This study includes electrophoretically enhanced sedimentation modeling for understanding the transport-rate parameter.

• **University of Washington**, Seattle, WA: a 36-month $197,089 grant for "Reduction of Inherent Mercury Emissions in PC Combustion." Dr. J. Kramlich will investigate (1) the reaction order of Hg with HCl, (2) free-radical enhancement; (3) the role of ash aerosols of varying compositions (generated by artificial char combustion) on the retention of oxidized mercury; and (4) treating coal to change aerosol yield on mercury capture.

• **Washington University**, St. Louis, MO: a 36-month $399,999 grant for "Novel Techniques for Slurry Bubble Column Hydrodynamics." M. Dudukovic will investigate the economic demands for quantification of slurry bubble column reactors (SBCR) hydrodynamics and scale-up. The research will (1) verify the computer-automated radioactive particle-tracking computer-assisted tomography (CARPT-CT) technique and develop a normal-pressure data base; (2) refine the constitutive equations (e.g., drag, interfacial interactions, turbulence) to align model predictions with data; and (3) use the models to predict the flow and holdup field at high pressure. The results will facilitate the design and scale-up of SBCR.

• **Yale University**, New Haven, CT: a 36-month $200,000 grant for "Advanced Solids NMR Studies of Coal Structure and Chemistry". A new solid-state NMR method will be developed for chemical analysis of coal structure. Dr. K. Zilm will investigate the differences in gas-prone and oil-prone coals by determining (1) the exchangeable hydrogens; (2) the nitrogen-containing organic functional groups; and (3) the micropore structure of coal, using laser-polarized 129Xe gas as an NMR probe. The results will be correlated with petrographic, depositional, geological-history, and other measures of coal structure.

Program Goal

The UCR goal is to promote the environmentally responsible, increased use of fossil fuels. This is vital to DOE's mission: it provides the foundation for industrial competitiveness, clean energy research, and improved environmental management.

A key priority is student education and training. Each research team must include at least one university student, compensated from the grant, and a teaching professor.

Project Benefits

The benefits of the University Coal Research Program are twofold:

• It sustains a national program of university research in fundamental coal studies.

• It helps to ensure a future supply of fossil energy scientists and engineers. More than 700 students have received science and engineering degrees with the help of Federal grants since the program's inception.

Research is restricted to U.S. colleges and universities—an ideal environment for fundamental research with high payoff potential in a competitive global economy.

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